

Butyl 3-methoxypropionate
4195-88-4 | DTXSID30194709

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 96.8 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.40e-01

Confidence level: 8.02e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethyl hexanoate</div> <div>Measured: 115</div> <div>Predicted: 110</div>	<div>Image not found</div> <div>2-Phenylethyl acetate</div> <div>Measured: 77.6</div> <div>Predicted: 98.8</div>	<div>Image not found</div> <div>Ethyl phenylacetate</div> <div>Measured: 77.6</div> <div>Predicted: 103</div>
<div>Image not found</div> <div>Aldicarb</div> <div>Measured: 31.6</div> <div>Predicted: 38.0</div>	<div>Image not found</div> <div>Ethyl heptanoate</div> <div>Measured: 407</div> <div>Predicted: 284</div>	